

Bioaccumulation Model Calibration Update

CPG-EPA Meeting

June 5, 2018

Topics

- Review of bioaccumulation memo regarding K_{OW} and K_D per memo from EPA
- Calibration status
 - Review of calibrated parameter values
 - Comparison with priority calibration metrics
- Verification of model calibration
 - Dynamic model runs
 - Results for 3rd chemical (1,2,3,4,6,7,8-HpCDF)
 - Running model for individual samples
- Next Steps

K_{OW} and K_D

- Agree with findings of May 17 memo...
 - Unsure that attempting to fix highly uncertain K_D value is advantageous.
 - Suggest that literature K_D values can be useful in verifying K_{OW}
- Calculated K_D at several K_{OW} values for LPRSA modeled fish/crab:

	K_D values for TCDD at various K_{OW} values				
	$K_{OW} = 5.5$	$K_{OW} = 6$	$K_{OW} = 6.5$	$K_{OW} = 7$	$K_{OW} = 7.5$
Range (large)	0.19-0.36	0.18-0.32	0.14-0.25	0.08-0.15	0.04-0.07
Range (small)	0.29-0.56	0.27-0.51	0.21-0.40	0.12-0.23	0.05-0.10
Average	0.33	0.30	0.24	0.14	0.06

- Suggests $K_{OW} \leq$ about 6.5 is more reasonable
 - Compare to range of literature values for K_D of TCDD found by EPA
 - $K_D = 0.12$ to 0.45 for rainbow trout

Calibration Process

- Identify sensitive parameters according to sensitivity analysis and previous model knowledge.
- Modify parameters in sequence, looping back as needed.
- Focus on priority calibration targets, while also looking at overall model performance.

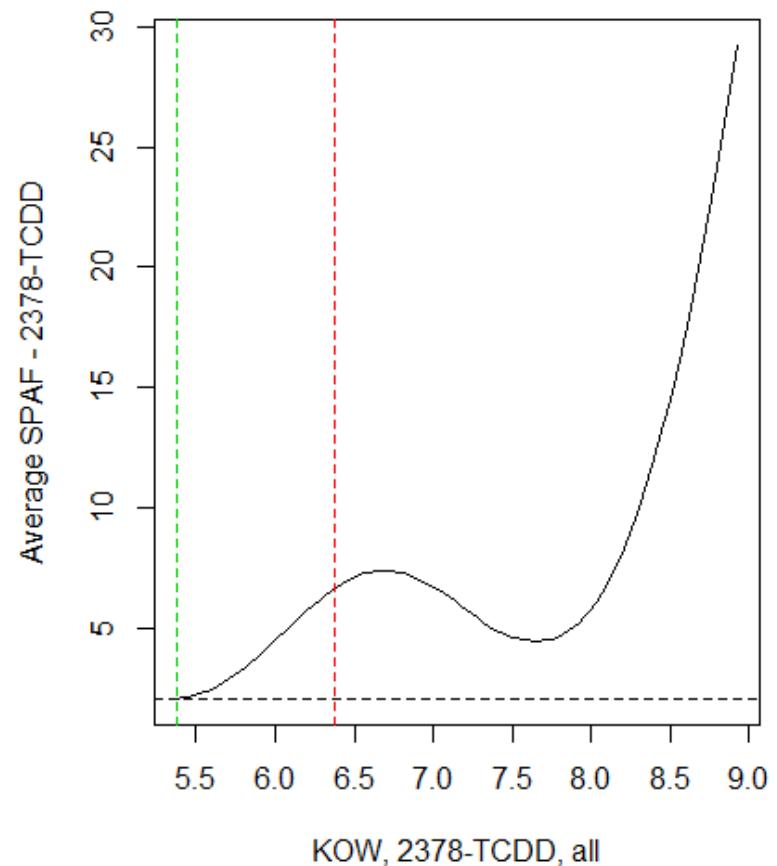
Reminder about Calibration Targets

Predictions relative to empirical tissue data:

Model Compartment	Count of Tissue Samples		
	RM 0 – 6	RM 6 – 14.7	RM 14.7 – 17.4
Benthic invertebrate DEPs	-	13	1
Benthic invertebrate C/Os	5	-	-
Small filter feeding fish	-	3	-
Small forage fish	11	13	1
Small American eel (< 50 cm)	3	6	5
Blue crab	19	21	4
Carp	na	11	3
Catfish	6	27	12
White perch	9	8	3
Large American eel (> 50 cm)	3	6	-
Bass	na	4	2

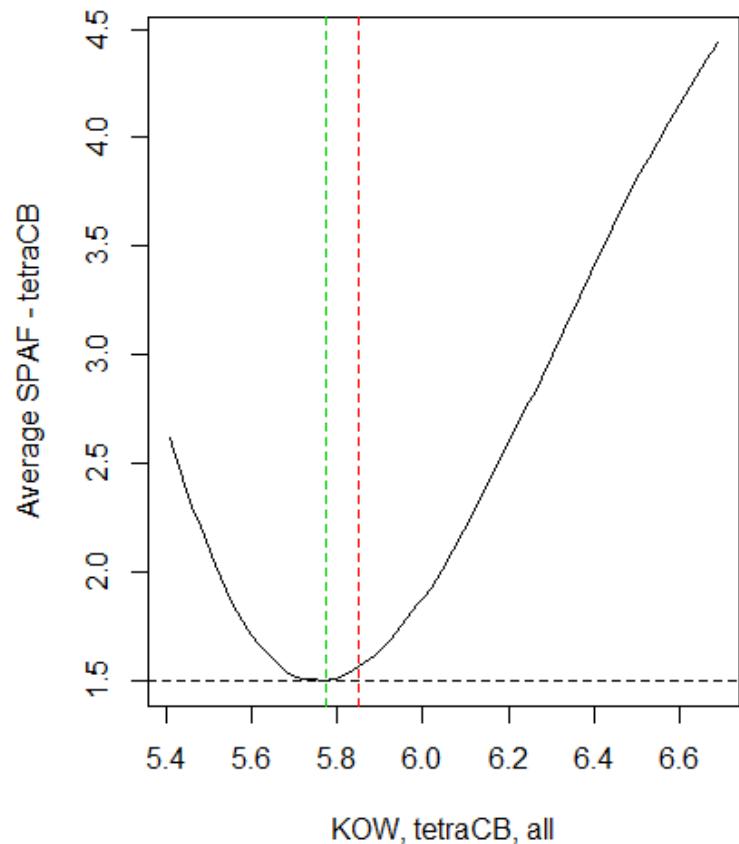
1 – K_{OW} for 2,3,7,8-TCDD

- Distribution
 - Nominal value = 6.38
 - Range = 5.38 to 8.93
- Optimization plot indicates best calibration at low-end of range (e.g., K_{OW} of 5.5).
- Alternative K_{OW} around 7.5 less desirable than originally thought.



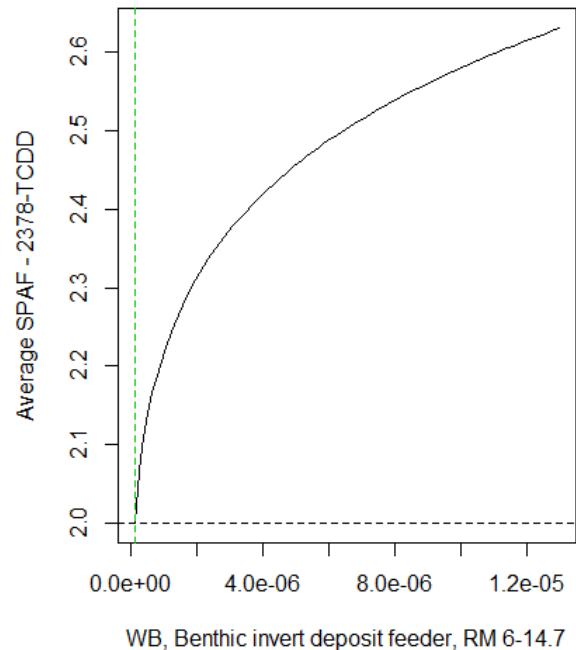
2 – K_{OW} for TetraCB

- Distribution
 - Nominal value = 5.85
 - Range = 5.38 to 6.65
- Initial optimization indicated K_{OW} of about 5.6.
- Revised optimization plot indicates best calibration at K_{OW} of about 5.75



3 - Weight of Benthic Deposit Feeding Invertebrates (RM 6-14.7)

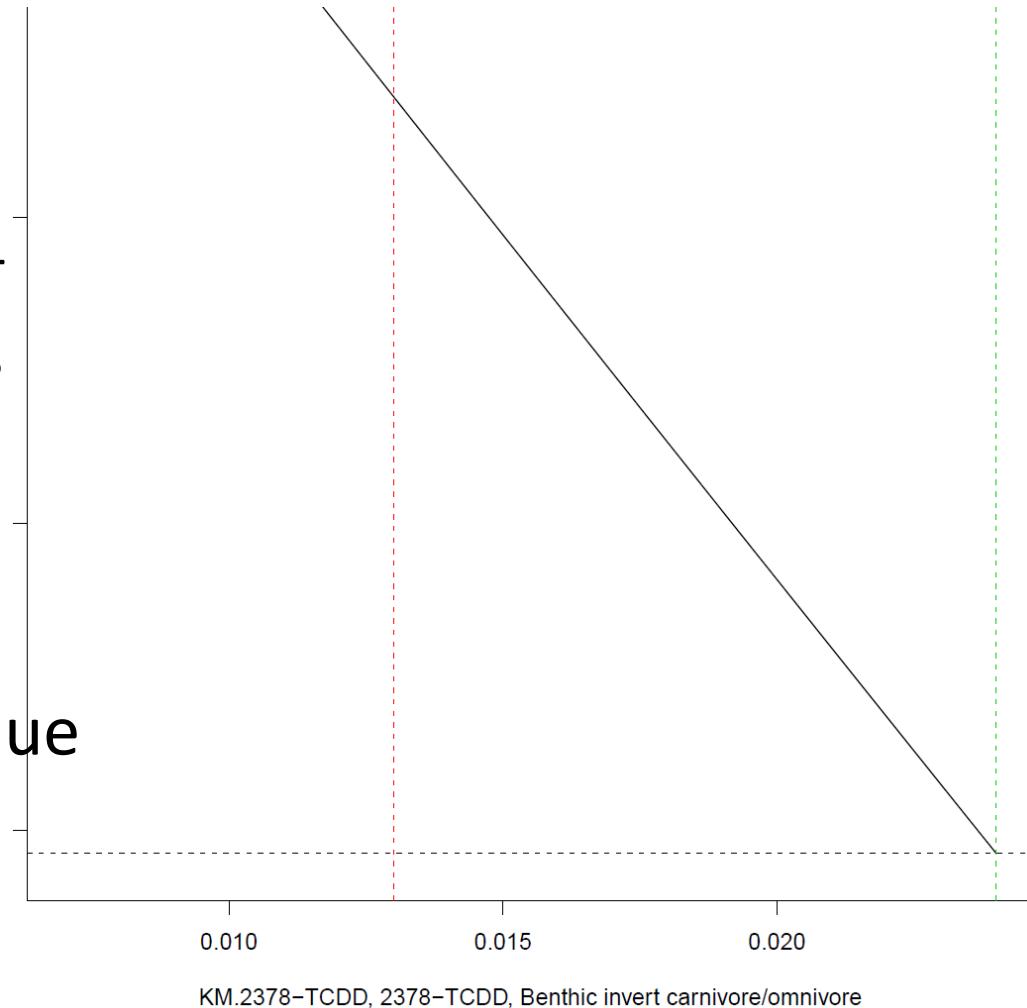
- Distribution
 - Nominal value = 36 mg ww
 - Range = 0.12 to 400 mg ww
- Optimization plot indicates lower values will result in improved SPAF.
- Selected calibrated value of 1 mg ww (1E-06 kg ww)
 - Better represents majority of species in this area.
 - Average skewed by several larger organisms.



Taxon ^a	Percent of Biomass By Modeling Zone ^b			Body Weight (mg ww) ^c
	RM 0-6	RM 6-14.7	RM 14.7-Dam	
Arcteonais lomondi		6%		1.11
Heteromastus filiformis	2%			3.31
Ilyodrilus templetoni		10%		0.95
Limnodrilus hoffmeisteri	1%	49%	3%	0.17
Limnodrilus udekemianus		10%	1%	1.83
Lumbriculidae		8%	95%	404
Macoma balthica	97%	1%		151
Quistadrilus multisetosus		9%		0.12
Slavina appendiculata		5%		1.11

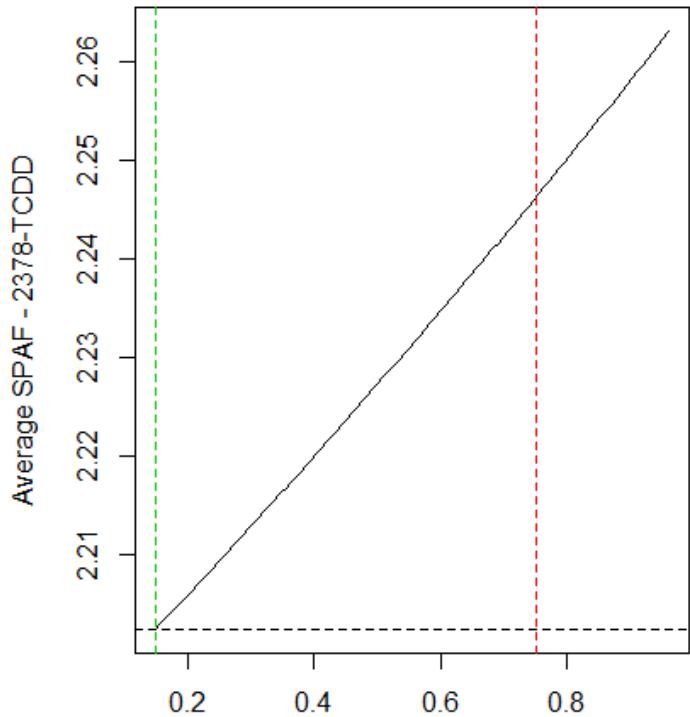
4 - Metabolic rate for invertebrates (2,3,7,8-TCDD)

- Distribution
 - Nominal value = 0.013
 - Range = 0.007 to 0.024
- Optimization indicates higher metabolic rate improves model performance.
- Selected calibrated value of 0.024 (max)



5 - Dietary AE of NLOC and NLOM for invertebrates (all types)

- Distribution
 - Nominal value = 0.75
 - Range = 0.15 to 0.96
- Optimization plot indicates lower values will result in improved SPAF (similar story with all related parameters).
- Selected value = 0.4 (based on previous conversations with Frank Gobas during 2015 calibration)



eP, Benthic invert deposit feeder, all

6 - Diet of Benthic Deposit Feeding Invertebrates (RM 6-14.7)

- Distribution:

Prey Items	RM 0 to RM 6		RM 6 to RM 14.7		RM 14.7 to RM 17.4	
	Nominal Value and Range (%)	Calibrated Value (%)	Nominal Value and Range (%)	Calibrated Value (%)	Nominal Value and Range (%)	Calibrated Value (%)
Sediment solids	23 (0 – 40)	23%	89 (70 – 100)	70%	84 (60 – 100)	70%
Particulates/detritus (near-bottom/fluff layer)	43 (25 – 75)	43%	10 (0 – 30)	26%	16 (0 – 40)	30%
Phytoplankton/algae	17 (0 – 30)	17%	0.5 (0 – 5)	2%	0 (0 – 5)	0%
Zooplankton	17 (0 – 30)	17%	0.5 (0 – 5)	2%	0 (0 – 5)	0%

- Optimization results:

- For RM 6-14.7 and RM 14.7 – Lower percentage of sediment and higher percentage of near-bottom particulates improves SPAFs.
- For RM 0-6 – Less important to model performance; no changes to nominal values.

7 - Dissolved Oxygen Saturation (RM 6-14.7)

- RM 0-6 and RM 14.7-Dam:
 - Relatively small range for RM 0-6 and RM 14.7-Dam
 - No changes to nominal values.
- RM 6-14.7 –
 - Optimization indicates that lower parameter values will improve SPAF.
 - Selected value of 80%.

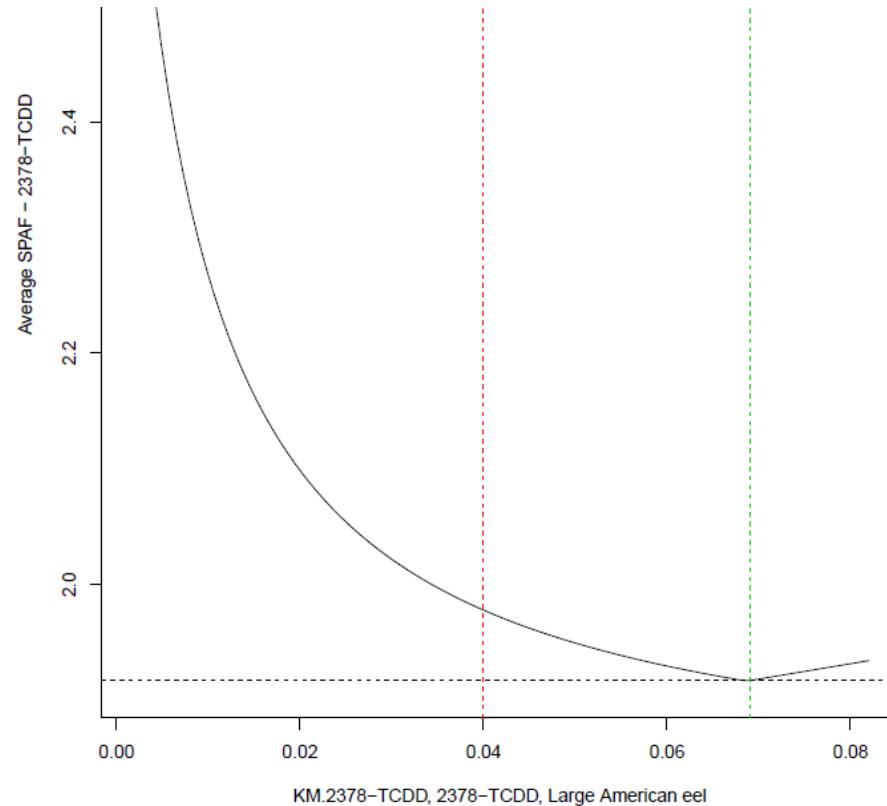
River Mile/ Modeling Area	DO Saturation (%)	
	Measured	Interpolated
RM 0-1	69%	-
RM 1-2	66%	-
RM 2-3	-	65%
RM 3-4	-	64%
RM 4-5	63%	-
RM 5-6	64%	-
RM 6-7	-	71%
RM 7-8	-	77%
RM 8-9	84%	-
RM 9-10	83%	-
RM 10-11	-	86%
RM 11-12	-	89%
RM 12-13	92%	-
RM 13-14	-	95%
RM 14-15	97%	-
RM 15-16	-	97%
RM 16-17.5	-	97%

Values by Modeling Area for Use in the Bioaccumulation Model:

RM 0 to RM 6	65% (64 – 69%)
RM 6 to RM 14.7	85% (71 – 97%)
RM 14.7 to RM 17.4	95% (92 – 97%)

8 - Metabolic rate for American eel (2,3,7,8-TCDD)

- Distribution:
 - Nominal value = 0.04
 - Range = 0.0016 to 0.082
- Optimization indicates improved model performance with higher values.
- Selected value of 0.06



9 - Lipid fraction for Benthic Invertebrate C/O for RM 0 – 6

- Distribution:
 - Nominal value = 1.6%
 - Range = 0.59% to 1.7%
- Optimization indicates improved model performance with lower values.
- Selected value of 0.6%

10 – Metabolic rate for carp (2,3,7,8-TCDD)

- Distribution:
 - Nominal value = 0.014
 - Range = 0.0016 to 0.056
- Optimization indicates improved model performance with value lower than nominal value.
- Selected value of 0.007 (half of nominal value)

11 – Diet for white perch (all areas)

- Distribution for percent of invertebrates in diet:

Diet component	Nominal Value	Range
Invertebrates	75%	0 – 100%
Small fish	15%	0 – 90%

- Optimization indicates improved SPAF with lower percentage of invertebrates and higher percentage of fish in diet.
- Selected values:
 - 40% invertebrates
 - 50% small fish

12 – Inputs from CFT model

- Modified inputs from CFT model
- Selected inputs to modify based on:
 - Sensitivity analysis
 - Contribution of inputs to predicted tissue concentrations
 - Model performance

Parameter	2,3,7,8-TCDD			TetraCB		
	RM 0-6	RM 6-14.7	RM 14.7-DD	RM 0-6	RM 6-14.7	RM 14.7-DD
Sediment	↑			↑		
Porewater						
Bioavailable water	↑			↑		
Fluff layer (near-bottom part.)	↑		↑	↑		
Water-column particulates						
Algal carbon						

13 – Water Temperature

- Distributions by area:

Area	RM 0 – 6	RM 6 – 14.7	RM 14.7 – Dam
Nominal value	12.7	13.0	13.4
Range of values	8 to 17	9 to 18	8 to 17

- Optimization indicated:
 - Higher temperature (i.e., higher bioaccumulation) better for RM 0-6 (both chemicals) and RM 14.7-Dam (TCDD)
 - Lower temperature (i.e., lower bioaccumulation) better for RM 6-14.7 (both chemicals) and RM 14.7-Dam (tetraCB)
- No change to parameter values

Calibration 1: Parameter values

Parameter	Nominal	Range	Selected	Min-----(Nominal)-----Max
1: K_{ow} for 2,3,7,8-TCDD	6.38	5.38 - 8.93	5.5	5.38  (6.38) ----- 8.93
2: K_{ow} for TetraCB	5.85	5.38 - 6.65	5.75	5.38 -----  (5.85) ----- 6.65
3: Weight of DEP (RM 6-14.7)	36 mg	0.12-400 mg	1 mg	0.12  (36) ----- 400
4: KM for inverts (2,3,7,8-TCDD)	0.013	0.007-0.024	0.024 (max)	0.007 ----- (0.013) ----- 0.024 
5: Invert dietary AE of NLOC/NLOM	0.75	0.15-0.96	0.4	0.15 -----  (0.75) ----- 0.9
6: % of sed in DEP diet (RM 6-14.7 and 14.7-Dam)	89%	70-100%	70% (min)	70% ----- (89%) ----- 100%
7: DO Saturation (RM 6-14.7)	85%	71-97%	80%	71% -----  (85%) ----- 97%

continued...

Parameter	Nominal	Range	Selected	Min-----(Nominal)-----Max
8: K_M for eel (2,3,7,8-TCDD)	0.04	0.0016-0.082	0.06	0.0016-----  ---(0.04)---  ---0.082
9: Lipid fraction for C/O (RM 0-6)	1.6%	0.59-1.7%	0.6% (min)	 ---59%-----  ---(1.6%)---1.7%
10: K_M for carp (2,3,7,8-TCDD)	0.014	0.0016-0.057	0.007	0.0016  ---(0.014)---0.057
11: % of inverts in WP diet	75%	0-100%	40%	0%-----  ---(75%)---100%
12: Sediment (RM 0-6); both chemicals			max	-----  ---(N)---
12: Fluff (RM 0-6); both chemicals			max	-----  ---(N)---
12: Water (RM 0-6); both chemicals			max	-----  ---(N)---
12: Fluff layer (RM 14.7-D); TCDD only			max	-----  ---(N)---

Calibration 1: Model performance

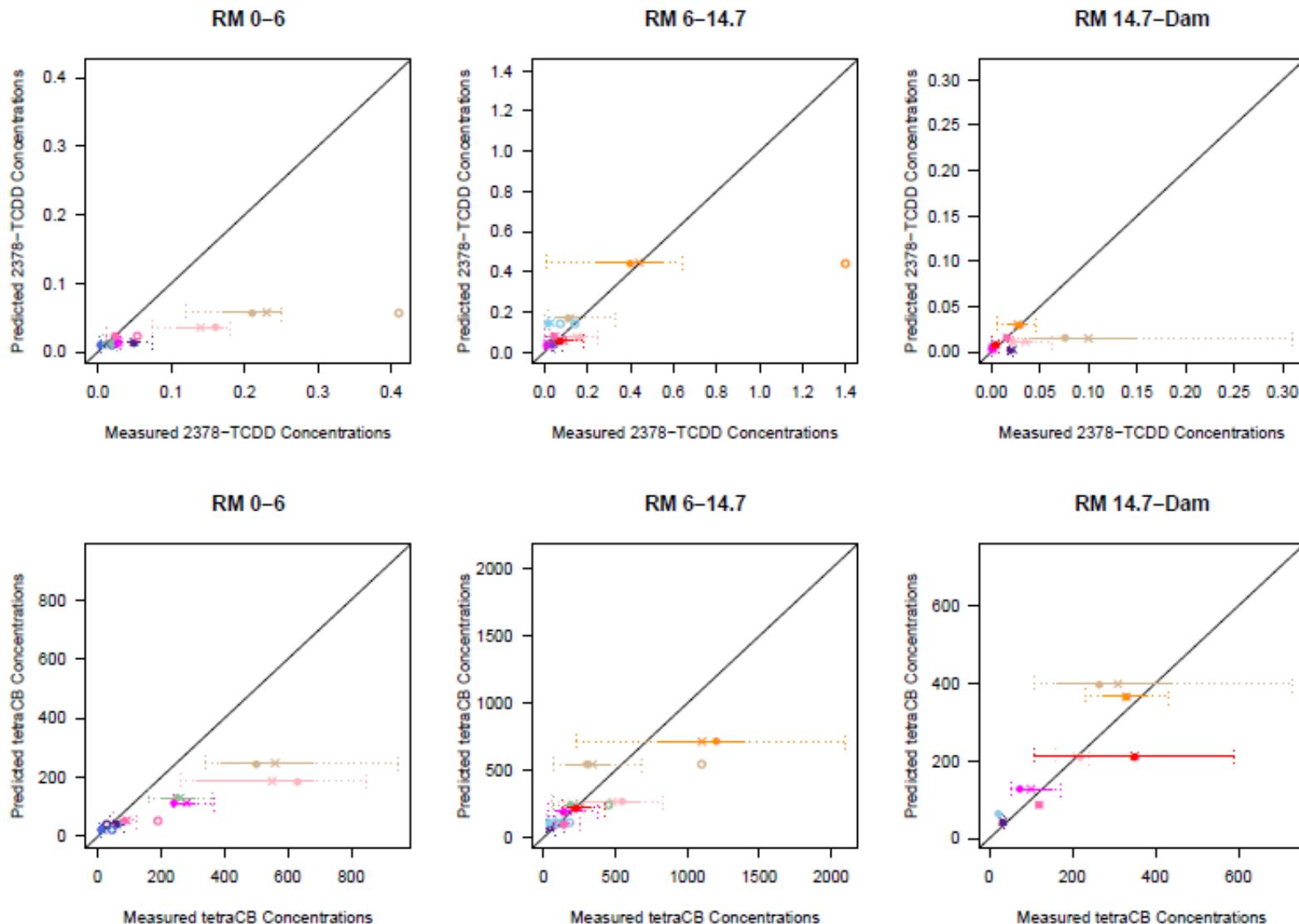
Uncalibrated Model Results

Species	2378-TCDD			TetraCB		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		50.6			6.0	
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	19.2			3.2		
Small filter feeding fish		2.8			-1.0	
Small forage fish	4.3	17.8	-2.1	-1.2	1.4	-1.4
Small American eel	2.0	22.6	4.1	-1.8	2.3	1.5
Blue crab	2.1	12.9	-6.5	1.1	3.5	1.7
Carp		1.1	-5.3		-1.2	1.2
Catfish	-1.8	5.5	-17.6	-1.6	2.8	1.4
White perch	-1.0	4.8	-6.0	-2.2	1.1	-1.2
Large American eel	3.0	8.3		-1.4	2.1	
Bass		7.9	1.3		1.9	-1.5
Average (all)	2.4	9.3	6.1	1.6	1.9	1.4
Average (priority)	8.4			2.0		

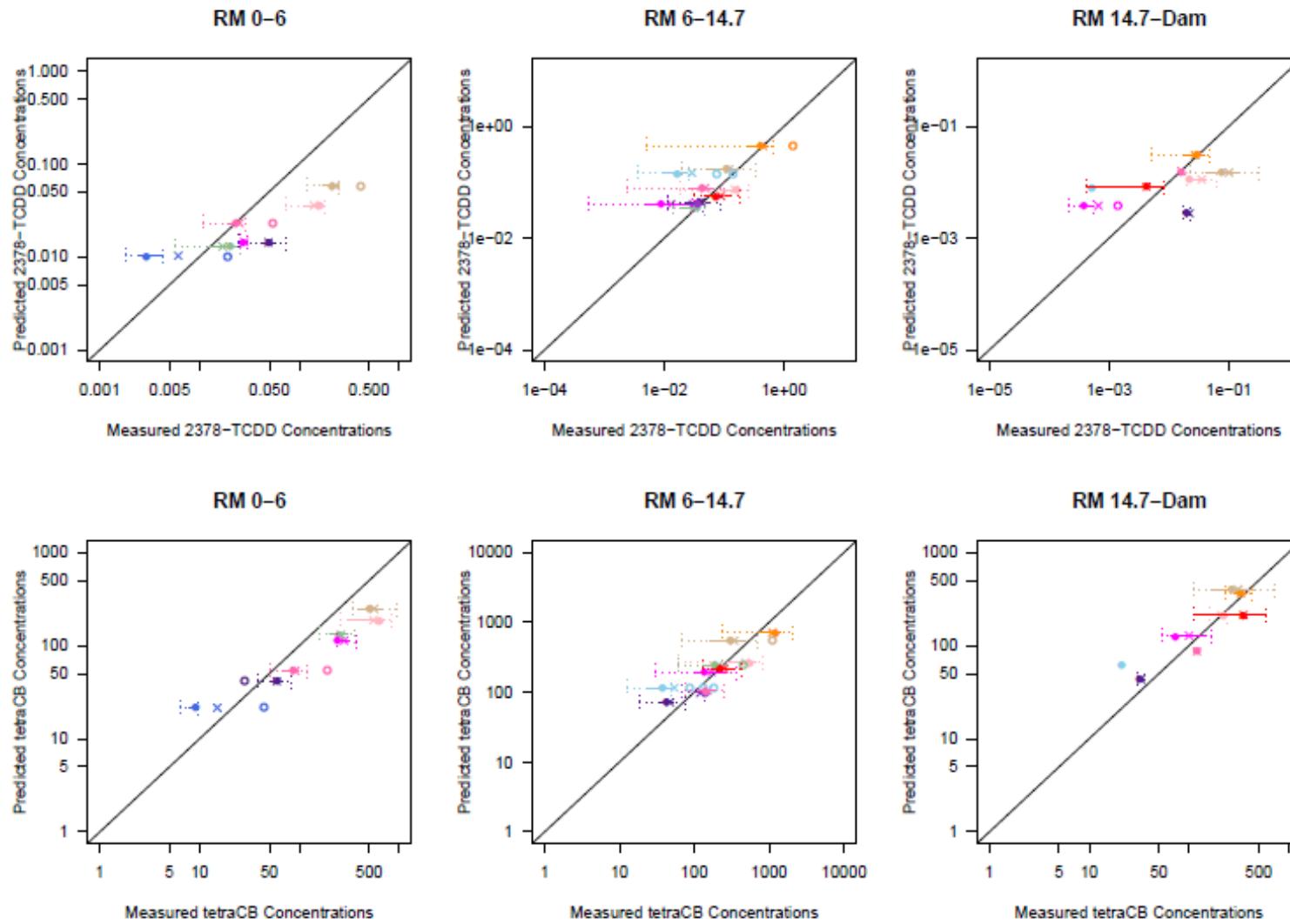
Calibration 1 Model Results

Species	2378-TCDD			TetraCB		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder				5.0		2.1
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore				1.7		1.4
Small filter feeding fish				1.4		-1.2
Small forage fish	-1.1	1.6		-1.0	-1.7	-1.4
Small American eel	-1.9	3.1		5.7	-2.5	1.1
Blue crab	-3.4	1.0		-7.9	-1.4	1.5
Carp				1.0	1.1	-1.5
Catfish	-4.0	1.4		-6.7	-2.3	1.6
White perch	-4.0	-2.0		-3.1	-2.9	-1.8
Large American eel	-1.3	1.1			-2.0	1.2
Bass		-1.6		2.0		-1.2
Average (all)	2.6	1.6	3.9	2.1	1.4	1.3
Average (priority)	2.0			1.6		

Calibration 1: Model performance



Calibration 1: Model performance



Calibration 2

- Consider alternative solution
- Start with addressing over-prediction in RM 6-14.7 modeling area for uncalibrated model.
 - Minimize key inputs from CFT model
 - Then look at results and proceed from there
- Results in model with higher K_{ow}

Calibration 2: Parameter values

Parameter	Nominal	Range	Selected	Min-----(Nominal)-----Max
Sediment (RM 6-14.7); 2,3,7,8-TCDD			min	★-----X-----)
Fluff (RM 6-14.7); 2,3,7,8-TCDD			min	★-----X-----)
Water (RM 6-14.7) ; 2,3,7,8-TCDD			min	★-----X-----)
Weight of DEP (RM 6-14.7)	36 mg	0.12-400 mg	0.12 mg (min)	★12 X (36)-----400
Invert dietary AE of NLOC & NLOM	0.75	0.15-0.96	0.4	0.15-----★-----X----- (0.75)-----0.96
% of sed in DEP diet (RM 6-14.7)	89%	70-100%	70%	★-----X----- (89%)-----100%
DO Saturation (RM 6-14.7)	85%	71-97%	80%	71%-----★-----X----- (85%)-----97%
K_{ow} for 2,3,7,8-TCDD	6.38	5.38 - 8.93	5.9	5.3 X ★ (6.38)-----8.93

continued...

Parameter	Nominal	Range	Selected	Min-----(Nominal)-----Max
K_M for inverts (2,3,7,8-TCDD)	0.013	0.007-0.024	0.02	0.007-----(0.013)-----  -----0.0 
K_M for eel (2,3,7,8-TCDD)	0.04	0.0016-0.082	0.08	0.0016-----(0.04)-----  -----0.8 
Fluff layer (RM 14.7-Dam); TCDD only			max	-----(N)----- 
K_{OW} for TetraCB	5.85	5.38 - 6.65	5.85	5.38-----  -----(5.85)-----6.65
Sediment (RM 0-6); both chemicals			max	-----(N)----- 
Fluff (RM 0-6); both chemicals			max	-----(N)----- 
Water (RM 0-6); both chemicals			max	-----(N)----- 

Calibration 2: Model performance

Uncalibrated Model Results

Species	2378-TCDD			TetraCB		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		50.6			6.0	
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	19.2			3.2		
Small filter feeding fish		2.8			-1.0	
Small forage fish	4.3	17.8	-2.1	-1.2	1.4	-1.4
Small American eel	2.0	22.6	4.1	-1.8	2.3	1.5
Blue crab	2.1	12.9	-6.5	1.1	3.5	1.7
Carp		1.1	-5.3		-1.2	1.2
Catfish	-1.8	5.5	-17.6	-1.6	2.8	1.4
White perch	-1.0	4.8	-6.0	-2.2	1.1	-1.2
Large American eel	3.0	8.3		-1.4	2.1	
Bass		7.9	1.3		1.9	-1.5
Average (all)	2.4	9.3	6.1	1.6	1.9	1.4
Average (priority)		8.4			2.0	

Calibration 2 Model Results

Species	2378-TCDD			TetraCB		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder				6.4		1.8
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	6.4				2.9	
Small filter feeding fish		2.1				-1.1
Small forage fish	2.1	2.5	1.6	-1.3	-1.2	-1.2
Small American eel	-1.5	2.8	6.0	-2.0	1.3	1.5
Blue crab	-1.4	1.8	-4.2	-1.1	1.7	1.6
Carp		-1.7	-1.3		-1.4	1.2
Catfish	-2.6	1.6	-5.1	-1.8	1.9	1.6
White perch	-2.0	-1.3	-2.3	-2.6	-1.8	-1.1
Large American eel	-1.0	1.0		-1.6	1.3	
Bass		1.2	3.7		1.1	-1.3
Average (all)	1.8	1.8	3.5	1.7	1.4	1.3
Average (priority)			1.7			1.5

Calibration 1 vs. 2 Performance

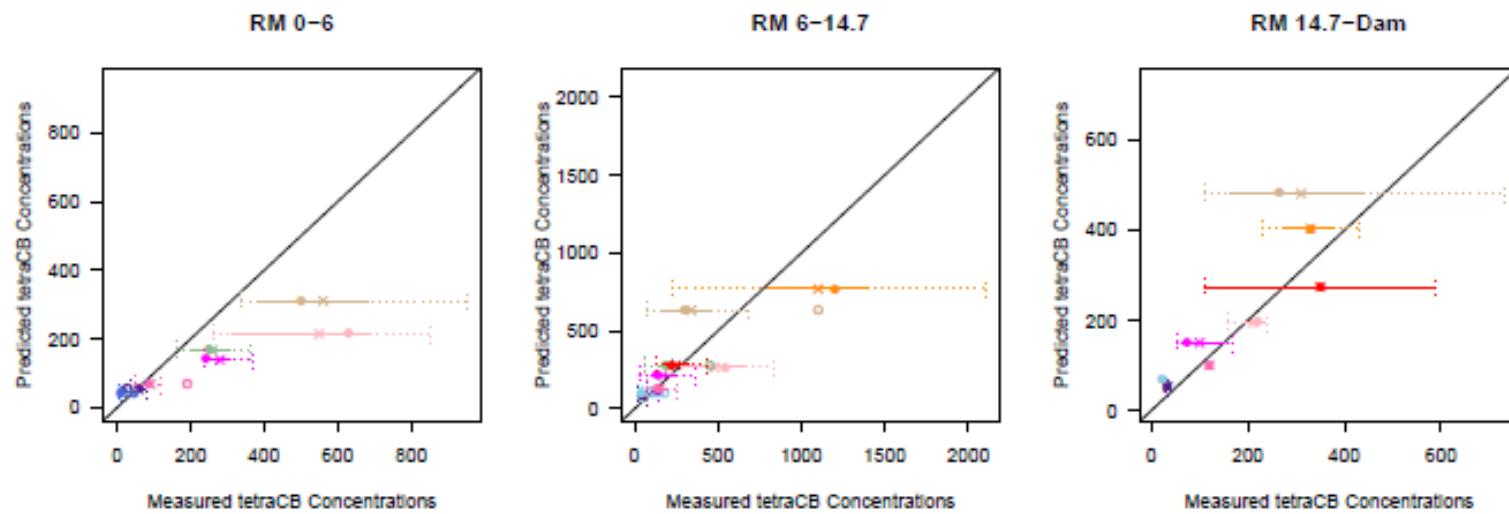
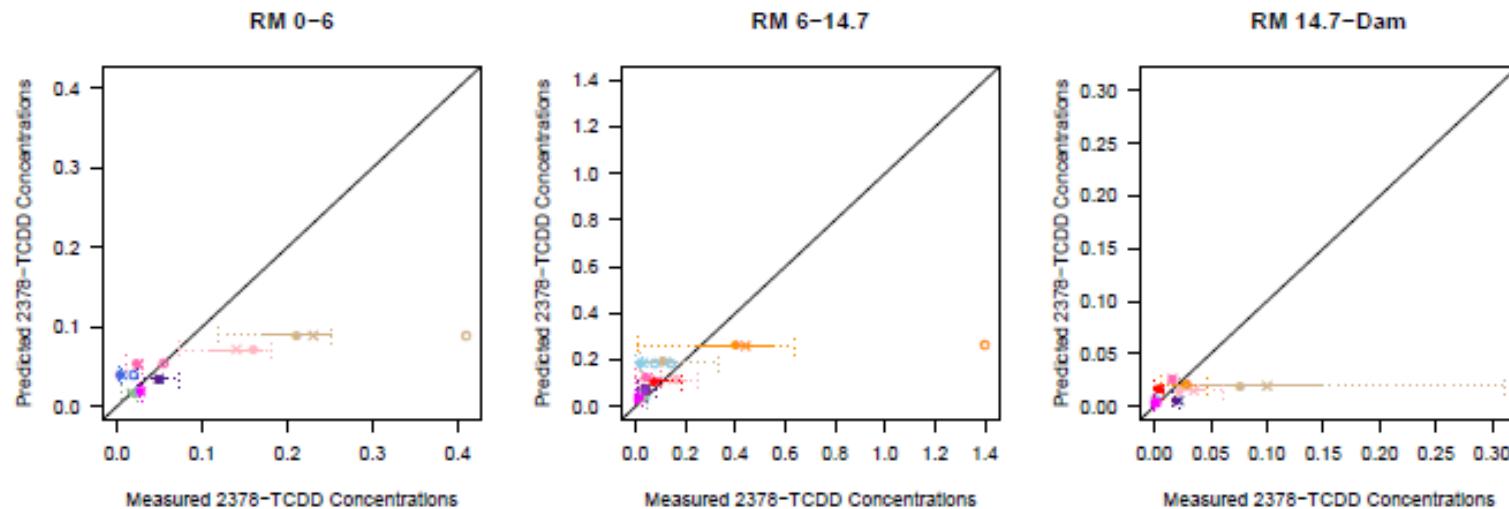
Calibration 1 Model Results

Species	2378-TCDD			TetraCB		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder		5.0			2.1	
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	1.7			1.4		
Small filter feeding fish		1.4			-1.2	
Small forage fish	-1.1	1.6	-1.0	-1.7	-1.4	-1.4
Small American eel	-1.9	3.1	5.7	-2.5	1.1	1.3
Blue crab	-3.4	1.0	-7.9	-1.4	1.5	1.3
Carp		1.0		1.1		-1.5
Catfish	-4.0	1.4		-6.7	-2.3	1.6
White perch	-4.0	-2.0		-3.1	-2.9	-1.8
Large American eel	-1.3	1.1			-2.0	1.2
Bass		-1.6	2.0		-1.2	-1.6
Average (all)	2.6	1.6	3.9	2.1	1.4	1.3
Average (priority)		2.0			1.6	

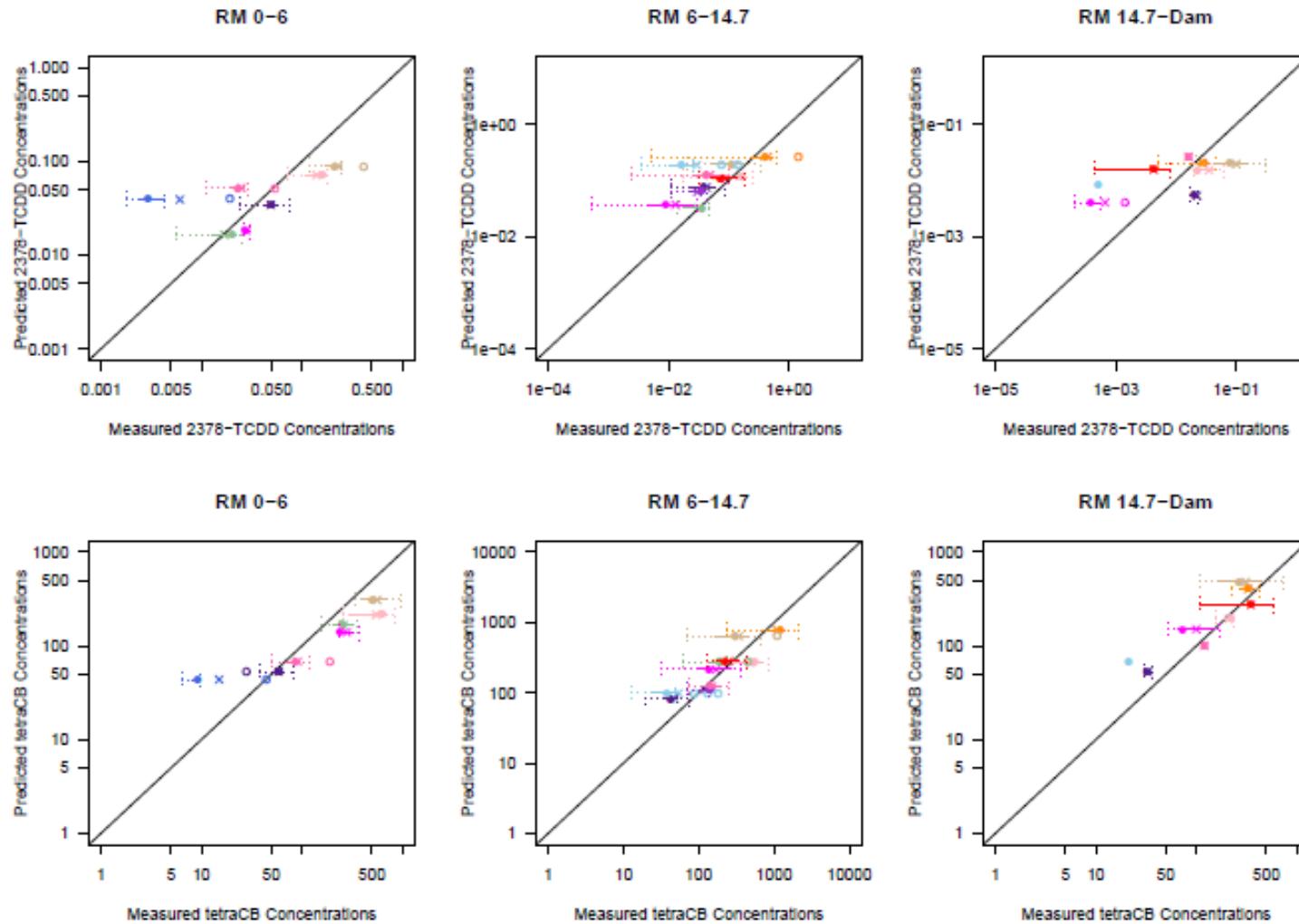
Calibration 2 Model Results

Species	2378-TCDD			TetraCB		
	RM 0-6	RM 6-14.7	RM 14.7-Dam	RM 0-6	RM 6-14.7	RM 14.7-Dam
Phytoplankton						
Zooplankton						
Benthic invert deposit feeder				6.4		1.8
Benthic invert filter feeder						
Benthic invert detritivore						
Benthic invert carnivore/omnivore	6.4				2.9	
Small filter feeding fish				2.1		-1.1
Small forage fish	2.1	2.5		1.6	-1.3	-1.2
Small American eel	-1.5	2.8		6.0	-2.0	1.3
Blue crab	-1.4	1.8		-4.2	-1.1	1.7
Carp				-1.7	-1.3	
Catfish	-2.6	1.6		-5.1	-1.8	1.9
White perch	-2.0	-1.3		-2.3	-2.6	-1.8
Large American eel	-1.0	1.0			-1.6	1.3
Bass				1.2	3.7	
Average (all)	1.8	1.8	3.5	1.7	1.4	1.3
Average (priority)				1.7		1.5

Calibration 2: Model performance



Calibration 2: Model performance

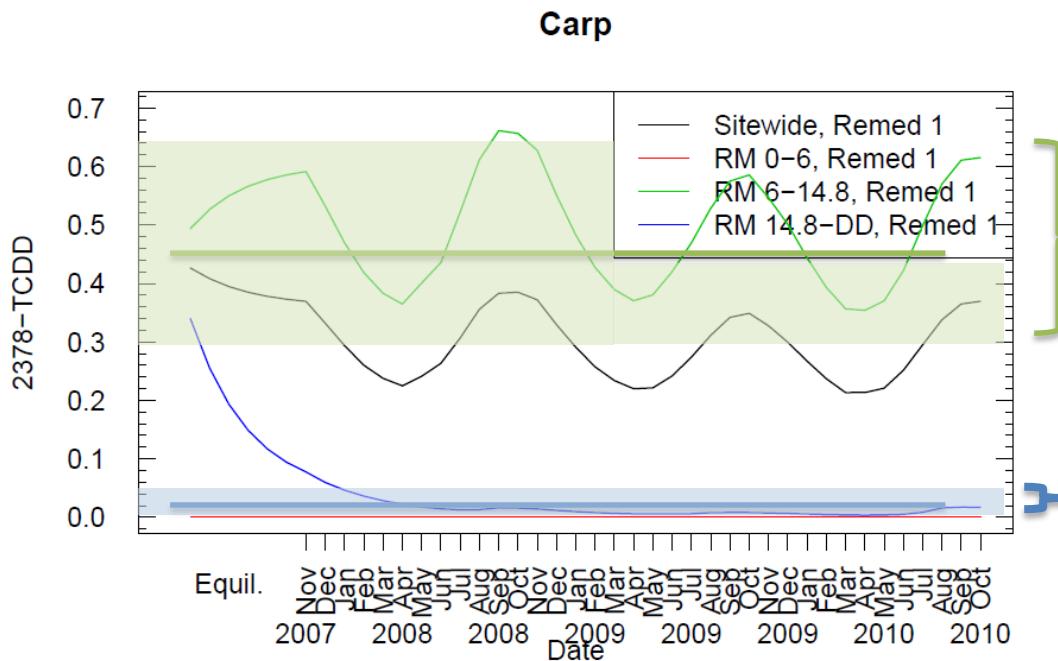


Model Verification

- 3rd chemical (1,2,3,4,6,7,8-HpCDF):
 - Currently working to finish parameterization
 - Will require some chemical-specific calibration
- Individual samples:
 - Initial results appears promising
 - Will look at data representativeness
- Dynamic model:
 - early runs look promising

Example of Dynamic Model Verification

- Calibration period (~3 years)
- Comparison of results produced by dynamic model with steady state model and empirical data.
- Example is for Calibration 1 – carp & 2,3,7,8-TCDD.



Empirical data

RM 6-14.7:
0.029 to 0.64, outlier
of 1.4 (n=10)

RM 14.7-Dam:
0.0052 to 0.046 (n=2)

Example of Model Evaluation for Individual Samples

- Preliminary model runs for calibration 1
- Carp & 2,3,7,8-TCDD
- Average SPAF:
 - RM 6-14.7 = 2.6
 - RM 14.7-Dam = 6.2

Composite ID	SPAF	Over / Under Prediction?
Modeling area: RM 6-14.7		
LPR3-CCWB-Ind005	2.3	-
LPR3-CCWB-Ind002	1.8	-
LPR4-CCWB-Ind175	1.4	-
LPR4-CCWB-Ind186	1.3	+
LPR5-CCWB-Ind011	1.1	-
LPR5-CCWB-Ind160	4.3	-
LPR6-CCWB-Ind028	1.9	+
LPR6-CCWB-Ind021	3.6	-
LPR7-CCWB-Ind042	1.6	+
LPR7-CCWB-Ind069	7.0	-
Modeling area: RM 14.7-Dam		
LPR8-CCWB-Ind139	1.2	-
LPR8-CCWB-Ind147	11.2	-

Next Steps

- Continue refining calibration
- Continue work on model verification steps:
 - Dynamic model
 - Model performance for individual samples
 - Model performance for 1,2,3,4,6,7,8-HpCDF
- Work on updating model documentation